

Ce²⁺ sensor based on naphthalen-1-yl-methylene-benzenesulfonohydrazide (NMBSH)

molecules: Ecological sample analysis

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New Journal of Chemistry: Electronic supplementary materials (ESM)

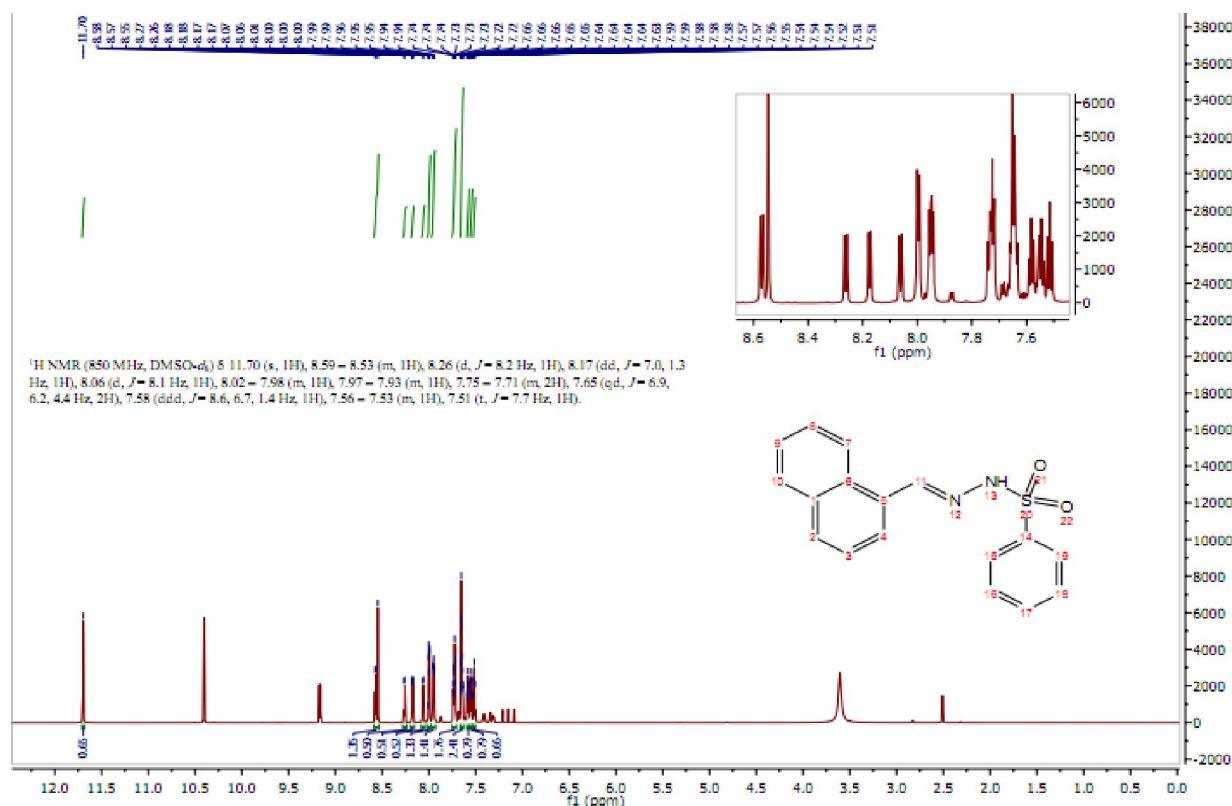


Figure S1: ¹H-NMR of NMBSH (4)

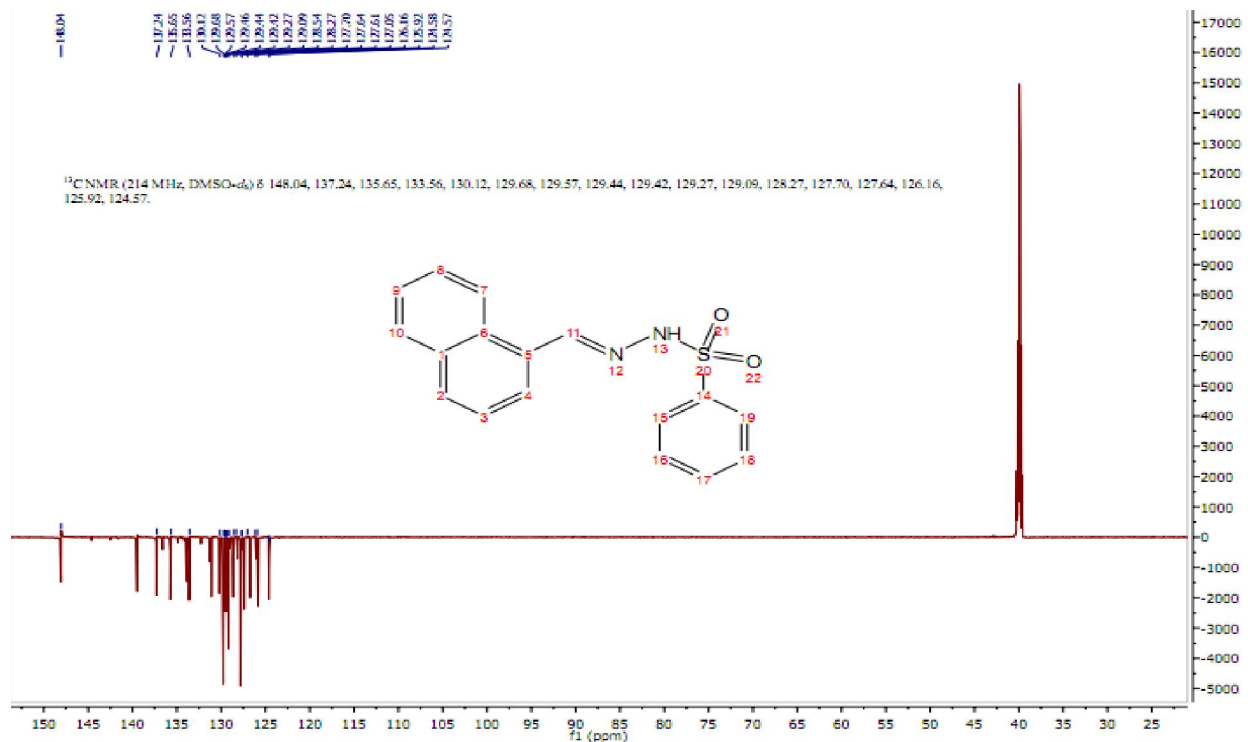


Figure S2: ^{13}C -NMR of NMBSH (4)

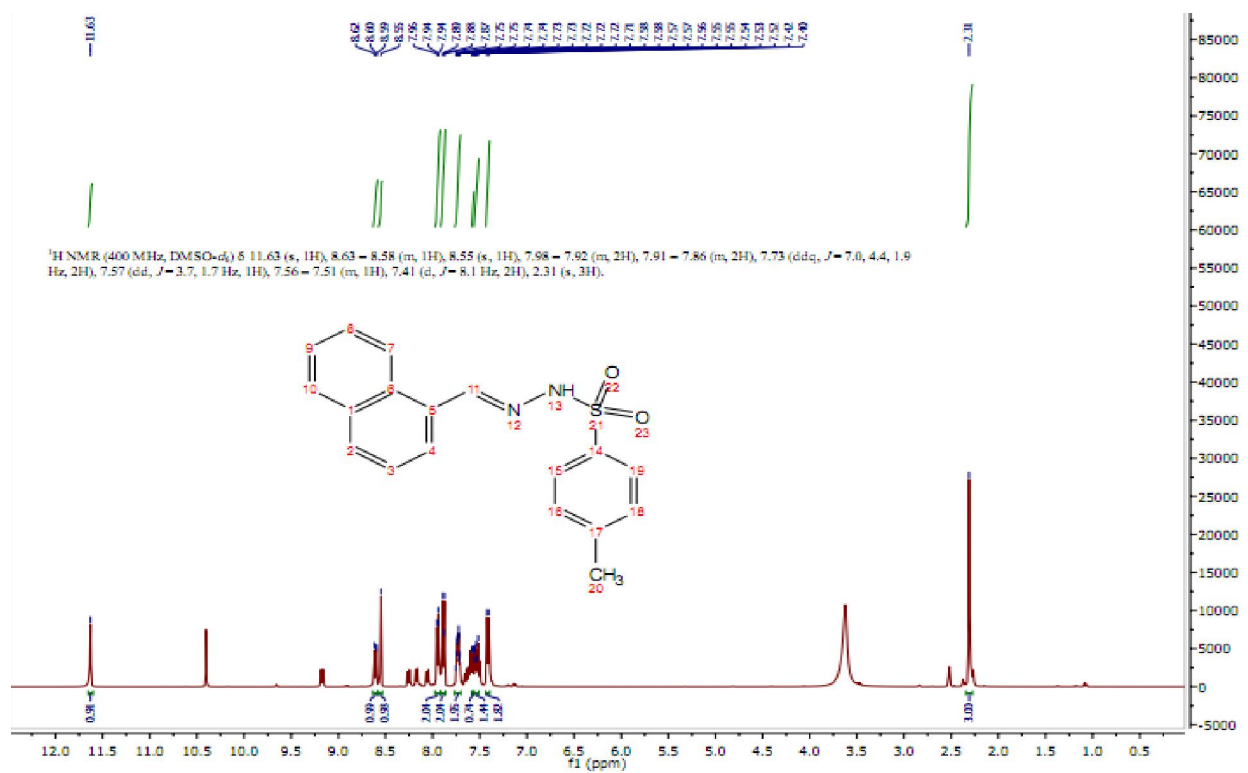


Figure S3: ^1H -NMR of NMBSH (5)

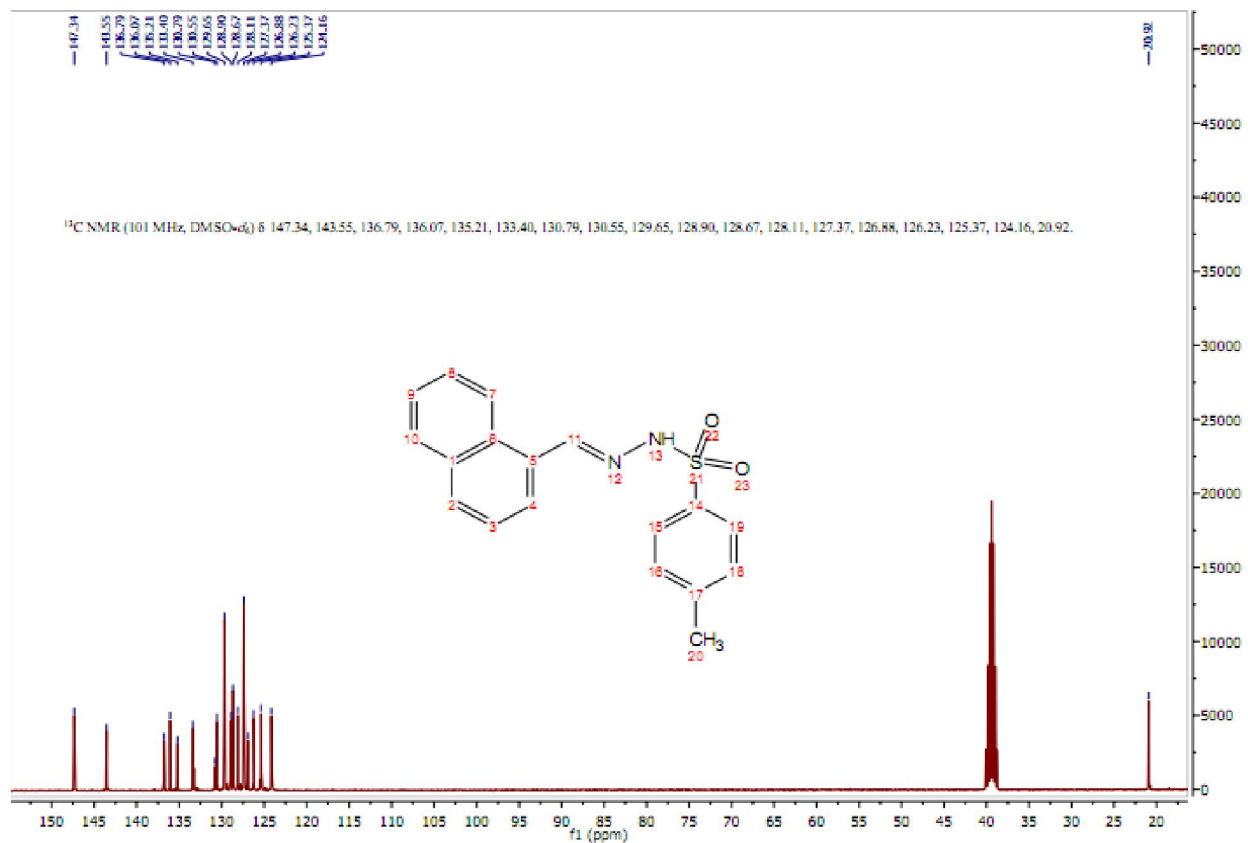


Figure S4: ¹³C-NMR of NMBSH (5)

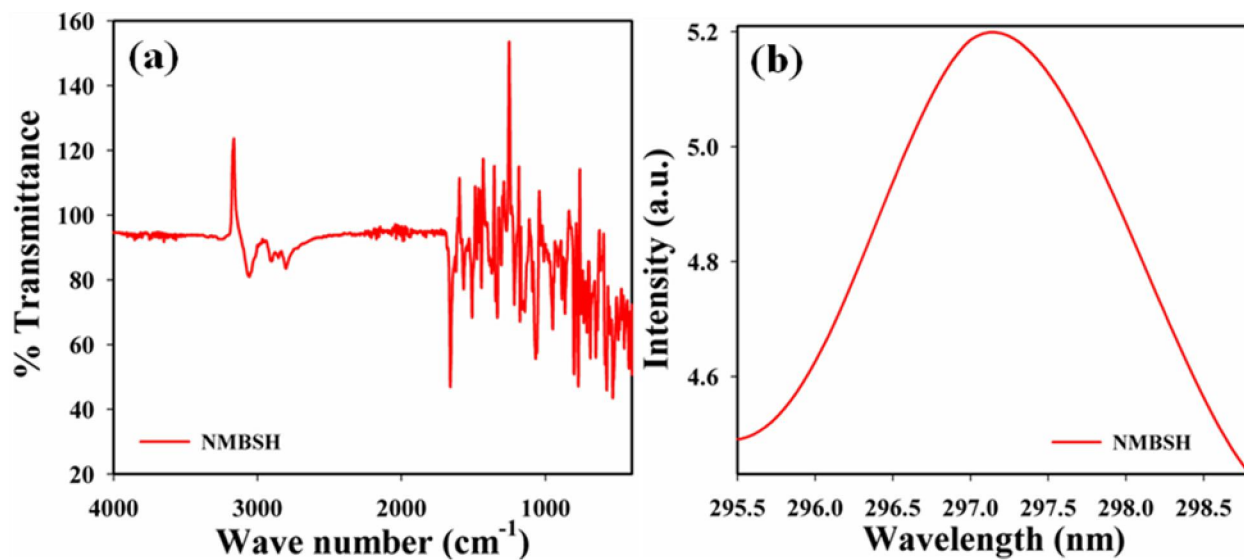


Figure S5: FTIR and UV spectra of NMBSH (4)

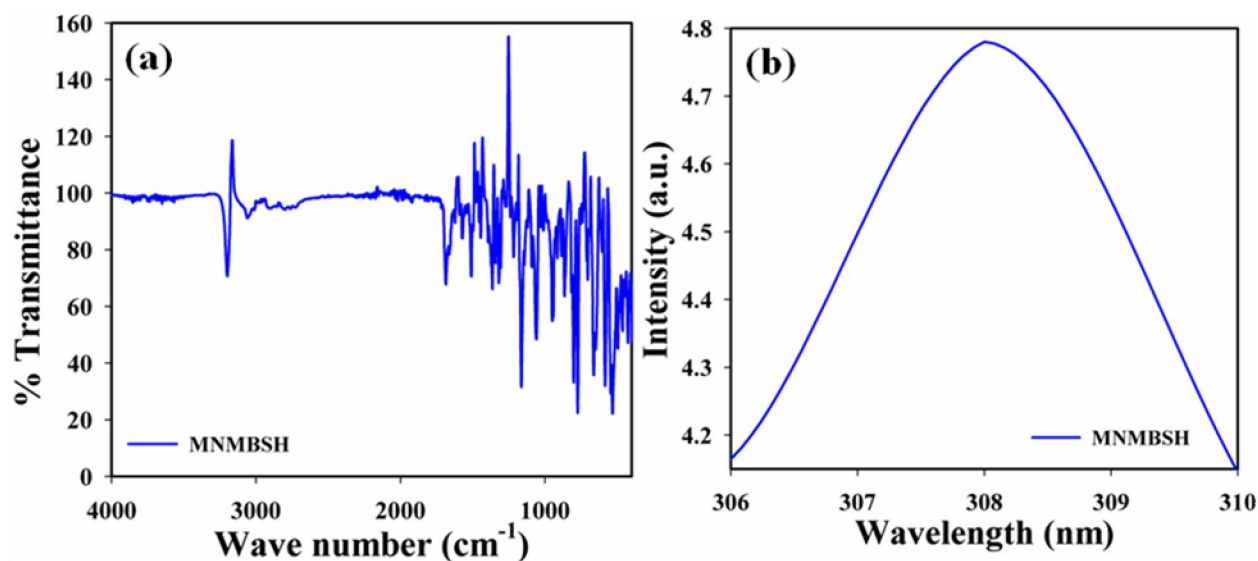


Figure S6: FTIR and UV spectra of MNMBSH (5)

Table S1: Bond Lengths for synthesized compounds

Atom	Atom	Length/Å	Atom	Atom	Length/Å
NMBSH (4)					
C1	C2	1.371(4)	C11	N1	1.270(3)
C1	C6	1.419(4)	C12	C13	1.364(5)
C1	C11	1.460(4)	C12	C17	1.377(4)
C2	C3	1.387(5)	C12	S1	1.749(3)
C3	C4	1.350(5)	C13	C14	1.375(5)
C4	C5	1.413(5)	C14	C15	1.364(6)
C5	C6	1.420(4)	C15	C16	1.370(6)
C5	C10	1.415(5)	C16	C17	1.380(6)
C6	C7	1.418(4)	N1	N2	1.403(3)
C7	C8	1.357(5)	N2	S1	1.630(3)
C8	C9	1.375(6)	O1	S1	1.424(2)
C9	C10	1.342(6)	O2	S1	1.421(2)
MNMBSH (5)					
C1	C2	1.379(3)	C12	C13	1.371(3)
C1	C6	1.424(3)	C12	C17	1.379(3)
C1	C11	1.461(3)	C12	S1	1.752(2)
C2	C3	1.389(3)	C13	C14	1.375(4)
C3	C4	1.357(4)	C14	C15	1.372(3)

C4	C5	1.415(3)	C15	C16	1.371(4)
C5	C6	1.418(3)	C15	C18	1.502(4)
C5	C10	1.408(3)	C16	C17	1.382(4)
C6	C7	1.424(3)	N1	N2	1.385(2)
C7	C8	1.360(3)	N2	S1	1.6276(19)
C8	C9	1.393(4)	O1	S1	1.4315(16)
C9	C10	1.350(4)	O2	S1	1.4234(17)
C11	N1	1.270(3)			

Table S2: Bond Angles for synthesized molecules

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
NMBSH (4)							
C2	C1	C6	119.1(3)	C13	C12	C17	121.0(3)
C2	C1	C11	115.5(3)	C13	C12	S1	120.8(2)
C6	C1	C11	125.4(3)	C17	C12	S1	118.2(3)
C1	C2	C3	122.2(4)	C12	C13	C14	120.6(3)
C4	C3	C2	119.5(4)	C15	C14	C13	119.0(4)
C3	C4	C5	121.7(4)	C14	C15	C16	120.4(4)
C4	C5	C6	118.4(4)	C15	C16	C17	121.0(4)
C4	C5	C10	122.7(4)	C12	C17	C16	117.9(4)
C10	C5	C6	118.9(4)	C11	N1	N2	115.7(3)
C1	C6	C5	119.0(3)	N1	N2	S1	114.0(2)
C7	C6	C1	124.1(3)	N2	S1	C12	107.33(14)
C7	C6	C5	116.8(3)	O1	S1	C12	107.06(15)
C8	C7	C6	121.3(4)	O1	S1	N2	106.95(14)
C7	C8	C9	121.4(4)	O2	S1	C12	110.27(15)
C10	C9	C8	119.6(4)	O2	S1	N2	104.52(16)
C9	C10	C5	121.8(4)	O2	S1	O1	120.03(14)
N1	C11	C1	124.7(3)				
MNMBSH (5)							
C2	C1	C6	119.22(19)	C13	C12	S1	120.73(17)
C2	C1	C11	119.9(2)	C17	C12	S1	120.14(18)
C6	C1	C11	120.88(18)	C12	C13	C14	119.9(2)
C1	C2	C3	121.8(2)	C15	C14	C13	122.2(2)
C4	C3	C2	120.2(2)	C14	C15	C18	121.6(3)

C3	C4	C5	120.6(2)	C16	C15	C14	117.2(2)
C4	C5	C6	119.6(2)	C16	C15	C18	121.2(2)
C10	C5	C4	121.1(2)	C15	C16	C17	121.8(2)
C10	C5	C6	119.2(2)	C12	C17	C16	119.8(2)
C5	C6	C1	118.53(18)	C11	N1	N2	115.52(17)
C5	C6	C7	117.7(2)	N1	N2	S1	116.70(14)
C7	C6	C1	123.80(19)	N2	S1	C12	107.06(10)
C8	C7	C6	120.8(2)	O1	S1	C12	107.47(10)
C7	C8	C9	120.9(2)	O1	S1	N2	107.00(10)
C10	C9	C8	120.0(2)	O2	S1	C12	109.64(11)
C9	C10	C5	121.3(2)	O2	S1	N2	103.84(10)
N1	C11	C1	120.92(19)	O2	S1	O1	121.00(11)
C13	C12	C17	119.1(2)				

Table S3: Reproducibility and repeatability study of NMBSH/GCE sensor

Replicates	Current (μA)	Reproducibility (%)		Current (μA)	Repeatability (%)	
		Individual	Average		Individual	Average
1	3.96	100		0.58	100	
2	1.71	43		0.52	90	
3	2.57	65	52	0.54	93	93
4	1.58	40		0.53	91	
5	1.09	28		0.54	93	
6	1.32	33		0.53	91	

Here, the reproducibility and repeatability of replicate 1 has been considered to be 100%.